

Abstracta

Ano IV - N.03



JUNEO2

Trabalhos Aceitos para Publicação em Periódicos.

- A 014 - 02 A proposal of quantum logic gates using cold trapped ions in a cavity.
- A 015 - 02 Studies on the anisotropic properties of MgB_2 .
- A 016 - 02 A possible correlation between suppression of superconductivity, magnetic ordering and normal state resistivity parameters in $Yb_{1-x}Pr_xBa_2Cu_3O_{7-\delta}$.
- A 017 - 02 Scaling laws in etched Si surfaces.

LIVRO PUBLICADO

L 002- 02 PREDICTIVE STATISTICAL MECHANICS: a Nonequilibrium Ensemble Formalism by Roberto Luzzi, Áurea R. Vasconcellos, and J. Galvão Ramos; ISBN: 1-4020-0482-6.

TRABALHOS PUBLICADOS MAIO/JUNHO 2002

P 025 -02 à P 057-02.

Trabalhos aceitos para publicação em Periódicos

A 014 - 02 A proposal of quantum logic gates using cold trapped ions in a cavity.

Semião F. L., Vidiella-Barranco A. and Roversi J. A.

We propose a scheme for implementation of logical gates in a trapped ion inside a high finesse cavity. The ion is interacting with a (classical) laser field as well as with the (quantized) cavity field. We demonstrate that simply by tuning the ionic internal levels with the frequencies of the fields, it is possible to construct a controlled-NOT gate in a three step procedure, having the ion's internal levels as well as vibrational (motional) levels as qubits. The cavity field is used as an auxiliary qubit and basically remains in the vacuum state.

Physics Letters A, accepted on May 2002

A 015 -02 Studies on the anisotropic properties of MgB_2 .

de Lima, O. F.

This paper presents a review on reported anisotropic properties of MgB_2 . The first direct measurement of an anisotropic superconducting property in MgB_2 was achieved for the bulk nucleation field H_{c2} , in samples of aligned crystallites. A ratio $H_{c2}^{ab} / H_{c2}^c \approx 1.7$ was found between the critical field parallel to the ab plane and parallel to the c axis direction. Further, detailed study of the H_{c2} angular dependence confirmed its bulk origin, in contrast with what would be expected for the surface nucleation field H_{c3} . A Fermi velocity anisotropy was evaluated to be $V_F^{ab} \approx 1.6 V_F^c$ assuming an isotropic order parameter. For an anisotropic s-wave pairing symmetry it has been estimated that $V_F^{ab} \geq 2.5 V_F^c$. Different H_{c2} anisotropy has been found by different authors, using different samples, measured in varied temperature ranges. Other reported anisotropic properties of MgB_2 in the superconducting state are the field penetration depth l , coherence length ξ , and energy gap D ; in the normal state are the magnetoresistance, compressibility, and thermal expansion. So far, most of the reported results have been obtained using aligned crystallites, c-axis oriented thin films and sub-millimeter crystals.

Brazilian Journal Physics, accepted on June 2002.

A 016- 02 A possible correlation between suppression of superconductivity, magnetic ordering and normal state resistivity parameters in $Yb_{1-x}Pr_xBa_2Cu_3O_{7-\delta}$.

A. Gupta, H. Narayan, P. N. Lisboa-Filho, C. A. Cardoso, F. M. Araujo-Moreira, O. F. de Lima and A. V. Narlikar

Polycrystalline samples of Pr doped $Yb_{1-x}Pr_xBa_2Cu_3O_{7-\delta}$ (i.e., Yb(Pr)-123) system for $0 \leq x \leq 1$ have been investigated for resistivity (ρ) and magnetization (M) as a function of temperature in normal and superconducting state. The gradual decrease in superconducting critical temperature $T_c(x)$ is shown to be correlated with the x dependent ratio of resistivity slope $(d\rho/dT)_{cc}$ (corresponding to the linear $\rho(T)$ region) and residual resistivity ρ_0 . Interestingly, a comparison of Yb(Pr)-123 with Y(Pr)-123 shows that the difference in the value of Pr concentration where this ratio tends to go to zero matches with the observed difference of x_c (critical Pr concentration where superconductivity is destroyed) in them. These observations seem consistent with a presence of dynamically fluctuating striped phase in them. We further discuss the possible origin of antiferromagnetic ordering of Pr ions for $x \geq x_c$.

Journal Modern Physics B, accepted on May 2002.

A 017 - 02 Scaling laws in etched Si surfaces.

Dotto, M. E. R., and Kleinke, M. U.

Self-affine scaling behavior of etched crystalline Si surfaces has been investigated by atomic force microscope. Si surface were etched by a small drop (few μL) of Na OH solution. Percolation characteristics were observed at the initial stages of Si (100) chemical etching. Roughness exponent (α) values increase with etching time, from 0.6 to 0.8, and the α functional behavior with respect to the etching power agrees with the Kessler-Levine-Tu model. Anomalous scaling behavior was characterized for etched Si(111) surfaces. The local value of the roughness exponent is associated to the diffusional process of plateaus growth. The global value of α is close to 0.4, a typical value for the Kardar-Parisi-Zang model, reflecting the highest growth rates on surfaces with higher slopes.

Physical Review B, accepted on June 2002.

ERRATA

Livro Publicado

L 002- 02 PREDICTIVE STATISTICAL MECHANICS: a Nonequilibrium Ensemble Formalism, by Roberto Luzzi, Áurea R. Vasconcellos, and J. Galvão Ramos; FUNDAMENTAL THEORIES OF PHYSICS 122 Kluwer Academic Pub. Group, February 2002, 344pp. ISBN:1-4020-0482-6.

PATENTES REGISTRADAS

PETROBRÁS S. A., PI N. 0106228-0, depositado em 23/12/2001. "Processo e Reator para Pirólise de Cargas Residuais", J. R. Gomes/Petrobrás, G. Ciampi e C. A. Luengo/UNICAMP.

Trabalhos Publicados

P 025 -02 "Atomic arrangement and conductance of metal nanowires".

Rodrigues, V. and Ugarte, D.

We have used high resolution transmission electron microscopy and mechanically controllable break junction technique to study metal NW structure and electrical transport properties. In the last stages just before rupture, gold and platinum nanowires are crystalline and defect-free. In particular, gold NWs assume merely three kinds of atomic arrangements, which were correlated to observed conductance behaviors

Physica Status Solidi B-Basic Research 230[2], 475-480. 2002.

P 026- 02 "Binding energy of charged excitons in semiconductor quantum wells in the presence of longitudinal electric fields".

Dacal, L. C. O. and Brum, J. A.

We present variational calculations of the binding energy for positively and negatively charged excitons (trions) in idealized GaAs/Al_{0.3}Ga_{0.7}As quantum wells with parabolic electrons and holes energy dispersions. The configuration interaction method is used with a physically meaningful single- particle basis set. We have shown that the inclusion of more than one electron quantum-well solution in the basis is important to obtain accurate values for the binding energies. The effects of longitudinal electric-field and quantum-well confinement on the charged excitons bound states are studied in the absence of magnetic field and the conditions for the trion ionization are discussed.

Physical Review B 65[11], art-115324. 2002.

P 027 -02 "Binding energy of charged excitons bound to interface defects of semiconductor quantum wells".

Dacal, L. C. O., Ferreira, R., Bastard, G., and Brum, J. A.

We present a model that takes into account the interface-defects contribution to the binding energy of charged excitons (trions). We use Gaussian defect potentials and one-particle Gaussian basis set. All the Hamiltonian defect terms are analytically calculated for the s-like trial wave functions. The dependence of the binding energy and of the trion size on the quantum-well width and on the defect size are investigated using a variational method for GaAs/Al_{0.3}Ga_{0.7}As quantum wells. We show that even in the case of strictly structural defects the trion is more strongly affected than the exciton.

Physical Review B 65[11], art-115325. 2002.

P 028 -02 "Comparison of different crystal forms of 3-dehydroquinase from Salmonella typhi and its implication for the enzyme activity".

Lee, W. H., Perles, L. A., Nagem, R. A. P., Shrive, A. K., Hawkins, A., Sawyer, L., and Polikarpov, I.

The type I 3-dehydroquinase dehydratase (DHQase) which catalyses the reversible dehydration of 3-dehydroquinic acid to 3-dehydroshikimic acid is involved in the shikimate pathway for the biosynthesis of aromatic compounds. The shikimate pathway is absent in mammals, which makes structural information about DHQase vital for the rational design of antimicrobial drugs and herbicides. The crystallographic structure of the type I DHQase from Salmonella typhi has now been determined for the native form at 1.78 Angstrom resolution (R=19.9%; R-free=24.7%). The structure of the modified enzyme to which the product has been covalently bound has also been determined but in a different crystal form (2.1 Angstrom resolution; R=17.7%; R-free=24.5%). An analysis of the three available crystal forms has provided information about the physiological dimer interface. The enzyme relies upon the closure of a lid-like loop to complete its active site. As the lid-loop tends to stay in the closed position, dimerization appears to play a role in biasing the arrangement of the loop towards its open position, thus facilitating substrate access

Acta Crystallographica Section D-Biological Crystallography 58, 798-804. 2002.

P 029 -02 "Crystallization kinetics: A solution for geometrical impingement".

Clemente, R. A. and Saleh, A. M.

Starting from the wrong derivation by Erukhimovitch and Baram of an equation alternative to the classical Kolmogoroff- Johnson-Mehl-Avrami one for the transformed fraction in an infinite specimen, undergoing an isothermal first-order phase transformation, it is shown that a different exact solution of the geometrical problem of impingement can be obtained. Such solution is equivalent to the empirical one already presented by Austin and Rickett more than sixty years ago and allows to better fit experimental results for isothermal transformations. This also suggests that perhaps different statistical derivations could allow to reach the same result.

Physical Review B 65[13], art-132102. 2002.

P 030 -02 "Effects of an electron gas on the negative trion in semiconductor quantum wells".

Dacal, L. C. O. and Brum, J. A.

We present here the results of calculations of the negative trion binding energy in the presence of an electron gas. The screening of the Coulomb interaction and the Pauli exclusion principle are considered. Our results show a rapid ionization of the negative trion due to the Pauli exclusion principle while the screening is mainly responsible for the weakening of the trion binding energy. (C) 2002 Elsevier Science B.V. All rights reserved

Physica E 12[1-4], 546-549. 2002.

P 031 -02 "Evidence for internal field in graphite: a conduction electron spin-resonance study".

Sercheli, M. S., Kopelevich, Y., da Silva, R. R., Torres, J. H. S., and Rettori, C.

We report on conduction electron spin-resonance measurements performed on highly oriented pyrolytic graphite samples between 10 and 300 K using $S(\nu = 4 \text{ GHz})$, $X(\nu = 9.4 \text{ GHz})$, and $Q(\nu = 34.4 \text{ GHz})$ microwave bands for the external de-magnetic field applied parallel (H parallel to c) and perpendicular (H perpendicular to c) to the sample hexagonal c-axis. The results obtained in the H parallel to c geometry are interpreted in terms of the presence of an effective internal ferromagnetic-like field, $H_{\text{eff}}(T, H)$, that increases as the temperature decreases and the applied dc-magnetic field increases. We associate the occurrence of the $H_{\text{eff}}(T, H)$ with the field-induced metal-insulator transition in graphite and discuss its origin in the light of relevant theoretical models. (C) 2002 Elsevier Science Ltd. All rights reserved

Solid State Communications 121[9-10], 579-583. 2002.

P 032 -02 "Extended state floating up in a lattice model: bona fide levitation fingerprints, irrespective of the correlation length".

Pereira, A. L. C. and Schulz, P. A.

The evolution of extended states with magnetic field and disorder intensities is investigated for 2D lattice models. The floating-up picture is revealed when the shift of the extended state, relative to the density of states, is properly taken into account, either for white-noise or correlated disorder. (C) 2002 Elsevier Science B.V. All rights reserved

Physica e 12[1-4], 650-653. 2002.

P 033 -02 "Hole concentration in a diluted ferromagnetic semiconductor".

dos Santos, R. R., Oliveira, L. E., and Castro, J. D. E.

We consider a mean-field approach to the hole-mediated ferromagnetism in III-V Mn-based semiconductor compounds in order to discuss the dependence of the hole density on that of Mn sites in $\text{Ga}_{1-x}\text{Mn}_x\text{As}$. The hole concentration, p , as a function of the fraction of Mn sites, x , is parametrized in terms of the product $m^*J(\text{pd})^2$ (where m^* is the hole effective mass and $J(\text{pd})$ is the Kondo like hole/local-moment coupling), and the critical temperature T_c . By using experimental data for these quantities, we have established the dependence of the hole concentration on x , which can be associated with the occurrence of a re-entrant metal-insulator transition taking place in the hole gas. We also calculated the dependence of the Mn magnetization on x , for different temperatures (T), and found that as T increases, the width of the composition-dependent magnetization decreases dramatically, and that the magnetization maxima also decrease in magnitude, indicating the need for quality control of the Mn doping level in diluted magnetic semiconductor devices

Journal of Physics-Condensed Matter 14[14], 3751-3757. 2002.

P 034 -02 "Influence of apolar group structure on the properties of Langmuir monolayers of polyphenyl carboxylic acids".

Dynarowicz-Latka, P., Kita, K., Milart, P., Dhanabalan, A., Cavalli, A., da Silva, D. A., dos Santos, M. C., and Oliveira, O. N.

Langmuir monolayers of purely aromatic carboxylic acids are investigated through surface pressure (π), surface potential (ΔV)-area (A) isotherms and Brewster angle microscopic studies. The monolayer characteristic of the basic compound, namely 5'-phenyl-1,1':3',1"-terphenyl-4-carboxylic acid, abbreviated as PTCA, is compared with its derivatives containing hydrophilic (nitro) or hydrophobic (phenyl) substituents attached to the symmetrical triphenyl-benzene core. The nature of the substituent as well as its position (2' or 4') has profound influence on the monolayer organization. Also, chemical modification leading to rotation restrictions of the hydrophobic moiety of PTCA was found to alter significantly its characteristic as Langmuir monolayer. The results are discussed in view of different orientation and different molecular packing arrangements. (C) 2002 Elsevier Science B.V. All rights reserved

Colloids and Surfaces A-Physicochemical and Engineering Aspects 198, 141-150. 2002.

P 035 -02 "Luttinger liquid superlattices: Realization of gapless insulating phases".

Silva-Valencia, J., Miranda, E., and dos Santos, R. R.

We investigate Luttinger liquid superlattices, periodic structures composed of two kinds of one-dimensional systems of interacting electrons. We calculate several properties of the low-energy sector: the effective charge and spin velocities, the compressibility, various correlation functions, the Landauer conductance, and the Drude weight. The low-energy properties are subsumed into effective parameters, much like homogeneous one-dimensional systems. A generic result is the weighted average nature of these parameters, in proportion to the spatial extent of the underlying subunits, pointing to the possibility of "engineered" structures. As a specific realization, we consider a one-dimensional Hubbard superlattice, which consists of a periodic arrangement of two long Hubbard chains with different coupling constants and different hopping amplitudes. This system exhibits a rich phase diagram with several phases, both metallic and insulating. We have found that gapless insulating phases are present over a wide range of parameters.

Physical Review B 65[11], art-115115. 2002.

P 036 -02 "Micro-photoluminescence of self-assembled quantum dots in the presence of an electron gas"

Nakaema, M. K. K., Brasil, M. J. S. P., Iikawa, F., Ribeiro, E., Heinzl, T., Ensslin, K., Medeiros-Ribeiro, G., Petroff, P. M., and Brum, J. A.

InGaAs/GaAs self-assembled quantum dots in the presence of a two-dimensional electron gas were studied by micro-photoluminescence. Several sharp optical emission lines attributed to individual quantum dots were observed. These lines exhibit a blue shift and a broadening as the electron gas density is increased. We discuss the origin of the blue shift considering the variation of the built-in electric field in the asymmetric geometry of the dots. The observed broadening of the quantum dot emission lines is an indication of coupling between the two-dimensional electron gas and the electrons in the quantum dot. (C) 2002 Elsevier Science B.V. All rights reserved

Physica e 12[1-4], 872-875. 2002.

P 037 -02 "Moisture adsorption by milk whey protein films"

Yoshida, C. M. P., Antunes, A. C. B., and Antunes, A. J.

Edible films, using whey protein as the structural matrix, were tested for water vapour diffusion properties. Whey protein films were prepared by dispersing 6.5% whey protein concentrate (WPC) in distilled water with pH kept at 7.0. Glycerol was the plasticizer agent. Film slabs (13.5 x 3.5 cm) were put in a chamber at 25°C and 75% relative humidity, being held in vertical planes for different periods of time. The mass gain was determined throughout the experiment. We show that moisture adsorption by milk whey protein films is well described by a linear diffusion equation model. After an adsorption experiment was performed the solution of the diffusion equation was fitted to the data to determine the diffusion coefficient of the material

International Journal of Food Science and Technology 37[3], 329-332. 2002.

P 038 -02 "Multichannel photomultiplier for multipass Thomson scattering diagnostics"

Monteiro, M. J. R., Machida, M., Daltrini, A. M., and Berni, L. A.

The application of a new multichannel 64 parallel amplification 10 stage photomultiplier arranged in 8 x 8 matrix of 20.32 mm x 20.32 mm, detector XP1752 from Philips, for laser light scattering diagnostics is now under development. Signal intensity calibration curve for eight parallel and individual channels, as well as cross talk between channels was measured. Also, Rayleigh scattering on nitrogen gas, normally used as optical calibration method for electron density measurements in Thomson scattering was realized, and the intensity of both detectors was compared making measurements with a tungsten lamp.

Brazilian Journal of Physics 32[1], 54-56. 2002.

P 039 -02 "Multiscale skeletons by image foresting transform and its application to neuromorphometry"

Falcao, A. X., Costa, L. D., and da Cunha, B. S.

The image foresting transform (IFT) reduces optimal image partition problems based on seed pixels to a shortest-path forest problem in a graph, whose solution can be obtained in linear time. Such a strategy has allowed a unified and efficient approach to the design of image processing operators, such as edge tracking, region growing, watershed transforms, distance transforms, and connected filters. This paper presents a fast and simple method based on the IFT to compute multiscale skeletons and shape reconstructions without border shifting. The method also generates one-pixel-wide connected skeletons and the skeleton by influence zones, simultaneously, for objects of arbitrary topologies. The results of the work are illustrated with respect to skeleton quality, execution time, and its application to neuromorphometry. (C) 2002 Pattern Recognition Society. Published by Elsevier Science Ltd. All rights reserved

Pattern Recognition 35[7], 1571-1582. 2002.

P 040 -02 "New short-wavelength laser emissions from optically pumped (CD3OD)-C-13"

Jackson, M., Hockel, H., Lauters, M., Vasconcellos, E. C. C., Allen, M. D., and Evenson, K. M.

We report the discovery of 15 new laser emissions from (CD3OD)-C-13 when optically pumped with a CW CO₂ laser. The wavelengths of these lines, ranging from 57.5 to 135.2 μm, are reported along with their polarization relative to the CO₂ PUMP laser, operating pressure and relative intensity. A three-laser heterodyne system was then used to measure the frequencies of 12 optically pumped laser emissions from this methanol isotope. These emissions range from 65.7 to 151.8 μm and are reported with fractional uncertainties up to $\pm 2 \cdot 10^{-7}$

IEEE Journal of Quantum Electronics 38[5], 429-431. 2002.

P 041 -02 "Pd on Cu(111) studied by photoelectron diffraction"

de Siervo, A., Soares, E. A., Landers, R., Fazan, T. A., Morais, J., and Kleiman, G. G.

The PdCu alloy system, which has important catalytic properties, has been the subject of many experimental and theoretical studies using a large number of different techniques. Theoretical and experimental structural studies converge in predicting ordered alloys for the Pd/Cu(1 1 0) and Pd/Cu(1 0 0) surfaces. No such agreement exists for the Pd/Cu(1 1 1) surface, however: indeed, few structural studies have been performed for this surface. Here, we report the first application of X-ray photoelectron diffraction (XPD) (using synchrotron radiation) in combination with LEED to determine the structure of ultra-thin epitaxial Pd films (similar to 1 ML) evaporated on Cu(1 1 1) single crystal surfaces. The analysis of the data was performed with the multiple scattering diffraction program of Chen and Van Hove. For the preparation condition used, a random surface alloy seems to form in the first three layers. The first interlayer distance expands whereas the second seems to contract. (C) 2002 Elsevier Science B.V. All rights reserved

Surface Science 504[1-3], 215-222. 2002.

P 042 -02 "Phase diagram of the anisotropic Kondo chain".

Novais, E., Miranda, E., Neto, A. H. C., and Cabrera, G. G.

We establish the phase diagram of the one-dimensional anisotropic Kondo lattice model at $T=0$ using a generalized two-dimensional classical Coulomb gas description. We analyze the problem by means of a renormalization group treatment. We find that the phase diagram contains regions of paramagnetism, partial and full ferromagnetic order

Physical Review Letters 88[21], art-217201. 2002.

P 043 -02 "Photochromic W-TiO₂ membranes".

Alcober, C., Alvarez, F., Bilmes, S. A., and Candal, R. J.

Journal of Materials Science Letters 21[6], 501-504. 2002.

P 044 -02 "Quantitative determination of metals in radish using x-ray fluorescence spectrometry".

Anjos, M. J., Lopes, R. T., Jesus, E. F. O., Simabuco, S. M., and Cesareo, R.

Using energy-dispersive X-ray fluorescence analysis with a Ti-filtered x-ray tube it was possible to determine the concentrations of several elements, such as K, Ca, Ti, Mn, Fe, Cu, Zn, Br, Rb, Sr, Zr and Pb, at ppm levels in radish plants (root and foliage) cultivated in soils treated with concentrations of 10, 20 and 30 t ha⁻¹ of organic compost from urban garbage. A significant increase was observed in the concentrations of K, Ca, Mn, Fe, Zn, Rb and Pb in radish plants cultivated in the treated soils in comparison with a control soil. The results suggest that radish plants can be used as bioindicator of contamination of agricultural soils. Copyright (C) 2002 John Wiley Sons, Ltd

X-Ray Spectrometry 31[2], 120-123. 2002.

P 045 -02 "Quenching of the exciton-spin relaxation via exchange interaction in GaAs/Al_xGa_{1-x}As quantum wells".

Urdanivia, J., Iikawa, F., Maialle, M. Z., Brum, J. A., Hawrylak, P., and Wasilewski, Z.

We studied the influence of the electron gas on the exciton spin relaxation in GaAs/AlGaAs quantum wells. We observed an increase of the continuous-wave degree of polarization and the exciton spin relaxation time with the electron density. These results are interpreted based on the quenching of the exciton bound state. As a consequence, the spin relaxation changes from one dominated by the long-range exciton exchange interaction for intrinsic excitonic transitions to one dominated by the hole spin relaxation when in the presence of the electron gas. The experimental results are in qualitative agreement with calculations of the exciton spin relaxation time in doped samples

Physical Review B 65[11], art-115336. 2002.

P 046 -02 "Stability and instability of polymorphic populations and the role of multiple breeding seasons in phase III of Wright's shifting balance theory".

de Aguiar, M. A. M., Sayama, H., Rauch, E., Bar-Yam, Y., and Baranger, M.

It is generally difficult for a large population at a fitness peak to acquire the genotypes of a higher peak, because the intermediates produced by allelic recombination between types at different peaks are of lower fitness. In his shifting-balance theory, Wright proposed that fitter genotypes could, however, become fixed in small isolated demes by means of random genetic fluctuations. These demes would then try to spread their genome to nearby demes by migration of their individuals. The resulting polymorphism, the coexistence of individuals with different genotypes, would give the invaded demes a chance to move up to a higher fitness peak. This last step of the process, namely, the invasion of lower fitness demes by higher fitness genotypes, is known as phase III of Wright's theory. Here we study the invasion process from the point of view of the stability of polymorphic populations. Invasion occurs when the polymorphic equilibrium, established at low migration rates, becomes unstable. We show that the instability threshold depends sensitively on the average number of breeding seasons of individuals. Iteroparous species (with many breeding seasons) have lower thresholds than semelparous species (with a single breeding season). By studying a particular simple model, we are able to provide analytical estimates of the migration threshold as a function of the number of breeding seasons. Once the threshold is crossed and polymorphism becomes unstable, any imbalance between the different demes is sufficient for invasion to occur. The outcome of the invasion, however, depends on many parameters, not only on fitness. Differences in fitness, site capacities, relative migration rates, and initial conditions, all contribute to determine which genotype invades successfully. Contrary to the original perspective of Wright's theory for continuous fitness improvement, our results show that both upgrading to higher fitness peaks and downgrading to lower peaks are possible

Physical Review E 65[3], art-031909. 2002.

P 047 -02 "Statistical characterization of the energy spectrum in 1D disordered multilayer systems".

Machado, E., Rey-Gonzalez, R. R., and Schulz, P. A.

Models of one dimensional systems with short range correlated disorder have predicted the existence of an energy region where the states are delocalized. This is contrary to the earlier belief that all the eigenstates are localized in 1D disordered systems. We study the statistical properties of the spectra of finite superlattices made up of short chains of random binary alloy which present correlated disorder.

Physica Status Solidi B-Basic Research 230[2], 343-346. 2002.

Trabalhos Publicados

P 048 -02 "Status of a hybrid three-neutrino interpretation of neutrino data".

Guzzo, M. M., de Holanda, P. C., Maltoni, M., Nunokawa, H., Tortola, M. A., and Valle, J. W. F.

We re-analyse the non-standard interaction (NSI) solutions to the solar neutrino problem in the light of the latest solar as well as atmospheric neutrino data. The latter require oscillations (OSC), while the former do not. Within such a three-neutrino framework the solar and atmospheric neutrino sectors are connected not only by the neutrino mixing angle θ_{13} constrained by reactor and atmospheric data, but also by the flavour-changing (FC) and non-universal (NU) parameters accounting for the solar data. Since the NSI solution is energy-independent the spectrum is undistorted, so that the global analysis observables are the solar neutrino rates in all experiments as well as the Super-Kamiokande day-night measurements. We find that the NSI description of solar data is slightly better than that of the OSC solution and that the allowed NSI regions are determined mainly by the rate analysis. By using a few simplified ansatzes for the NSI interactions we explicitly demonstrate that the NSI values indicated by the solar data analysis are fully acceptable also for the atmospheric data. (C) 2002 Elsevier Science B.V. All rights reserved

Nuclear Physics B 629[1-3], 479-490. 2002.

P 049 -02 "Structure and melting of Bi nanocrystals embedded in a B2O3- Na2O glass".

Kellermann, G. and Craievich, A. F.

A composite material consisting of spherical Bi nanoclusters (nanocrystals and/or liquid nanodroplets) embedded in a $28\text{Na}(2)\text{O}\cdot 72\text{B}(2)\text{O}(3)$ glass was studied by the wide-angle x-ray scattering (WAXS) and small-angle x-ray scattering (SAXS) techniques over the temperature range in which the Bi crystal-liquid transition occurs. Because of the wide radius distribution of Bi clusters and due to the dependence of the melting temperature on crystal radius, the overall transition occurs over a wide range, from 365 up to 464 K. In this transition range, large Bi nanocrystals coexist with small liquid droplets. A weak contraction in a and c lattice parameters of rhombohedral Bi nanocrystals with respect to the bulk crystal was detected. As expected, the average radius of crystalline Bi clusters, deduced from WAXS data, increases for increasing temperatures over the whole solid-to-liquid transition range. The SAXS spectrum recorded at different temperatures within the transition range is essentially invariant, indicating that the radius distribution of Bi nanoclusters (nanocrystals and nanodroplets) is temperature independent. The volume distribution of Bi nanoclusters is a single-mode function with the radius ranging from about 15 up to 41 Angstrom with a maximum at 28 Angstrom. The integral of Bragg peaks of Bi nanocrystals decreases for increasing temperatures as a consequence of the progressive melting of nanocrystals of increasing size. By combining the results of WAXS and SAXS experiments, we determined the melting temperature of the nanocrystals as a function their radius suppressing unwanted size dispersion effects. Our results clearly indicate a linear dependence of the melting temperature on nanocrystal reciprocal radius, thus confirming previous theoretical predictions

Physical Review B 65[13], art-134204. 2002.

P 050 -02 "Surface and interface states in the Cu/V(110) structure".

Legoas, S. B. and Laks, B.

We present ab initio calculations of the electronic structure of copper multilayers on V(110) surface. The calculations were based on density-functional theory and the real-space linear muffin-tin orbital method in the atomic-sphere approximation was used. Surface and interface states were investigated using the Green-function based transfer-matrix method. The results shown a variety of electronic states along the main symmetry lines of the two-dimensional Brillouin zone, and the presence of surface and interface states was verified. Also, the existence of a binding state about 1.8 eV below the Fermi level is in good agreement with recent photoemission experiments, such state can be interpreted as a quantum-well state

Physical Review B 65[11], art-113403. 2002.

P 051 -02 "Synthesis and properties of new molecule-based magnets containing Mn(II), Cu(II) and nitronyl nitroxide radical cation".

Vaz, M. G. F., Knobel, M., Speziali, N. L., Moreira, A. M., Alcantara, A. F. C., and Stumpf, H. O.

In this work, we describe the synthesis of two new copper(II) compounds, (Pr-Rad)(2) [Cu(opba)].H₂O (1) and (Bu-Rad)(2)[Cu(opba)].2H₂O (2) where opba stands for orthophenylenebis(oxamato) and R-Rad(+) are nitronyl nitroxide radical cations. From 1 and 2, two new molecule-based magnets [Pr-Rad](2)[Mn-2{Cu(opba)}(3)].3.3DMSO.5H₂O (3) and [Bu-Rad](2) [Mn-2{Cu(opba)}(3)].3DMSO.6H₂O (4) were obtained, respectively. The magnetic properties of precursors 1 and 2 show the presence of ferromagnetic interaction between the radical cations with copper(II), in the temperature range of 20-300 K. The magnets 3 and 4 exhibit spontaneous magnetization at critical temperatures, T_c, of 23 K and 24 K, respectively.

Journal of the Brazilian Chemical Society 13[2], 183-189. 2002.

P 052 -02 "The status of the Brazilian spherical detector".

Aguiar, O. D., Andrade, L. A., Camargo, L., Costa, C. A., de Araujo, J. C. N., Neto, E. C. D., de Souza, S. T., Fauth, A. C., Frajuca, C., Frossati, G., Furtado, S. R., Furtado, V. G. S., Magalhaes, N. S., Marinho, R. M., Matos, E. S., Meliani, M. T., Melo, J. L., Miranda, O. D., Oliveira, N. F., Ribeiro, K. L., Salles, K. B. M., Stellati, C., and Velloso, W. F.

The first phase of the Brazilian Graviton Project is the construction and operation of the gravitational wave detector Mario Schenberg at the Physics Institute of the University of Sao Paulo. This gravitational wave spherical antenna is planned to feature a sensitivity better than $h = 10^{-21}$ Hz^{-1/2} at the 3.0-3.4 kHz bandwidth, and to work not only as a detector, but also as a testbed for the development of new technologies. Here we present the status of this detector

Classical and Quantum Gravity 19[7], 1949-1953. 2002.

P 053-02 "Theoretical and experimental investigation of the electron spin resonance of Co^{2+} in Zn-2(OH)PO_4 and Mg-2(OH)AsO_4 ".

Foglio, M. E., dos Santos, M. C., Barberis, G. E., Rojo, J. M., Mesa, J. L., Lezama, L., and Rojo, T.

Electron spin-resonance experiments were performed on Co^{2+} substituting for Zn^{2+} or Mg^{2+} in powder samples of Zn-2(OH)PO_4 and Mg-2(OH)AsO_4 . These two compounds are iso-structural and contain the Co^{2+} in two environments with approximately octahedral and trigonal bipyramidal structures. The observed resonances are described using a theoretical model that considers the departures from the two perfect structures. It is shown that resonance in the penta-coordinated complex is allowed, and the crystal fields that would reproduce the resonance of the Co^{2+} in the two environments are calculated. The low intensity of the resonance in the penta-coordinated complex is explained by assuming that this site is much less populated than the octahedral one; this assumption was verified by a molecular calculation of the energies of the two environments, with both Co and Zn as central ions in Zn-2(OH)PO_4 .

Journal of Physics-Condensed Matter 14[8], 2025-2041. 2002.

P 054-02 "Theoretical studies of non inductive current drive in compact toroids".

Farengo, R., Lifschitz, A. F., Caputi, K. I., Arista, N. R., and Clemente, R. A.

Three non inductive current drive methods that can be applied to compact toroids are studied. The use of neutral beams to drive current in field reversed configurations and spheromaks is studied using a Monte Carlo code that includes a complete ionization package and follows the exact particle orbits in a self-consistent equilibrium calculated including tile beam and plasma currents. Rotating magnetic fields are investigated as a current drive method for spherical tokamaks by employing a two dimensional model with fixed ions and massless electrons. The time evolution of the axial components of the magnetic field and vector potential is obtained by combining an Ohm's law that includes the Hall term with Maxwell's equations. The use of helicity injection to sustain a flux core spheromak is studied using the principle of minimum rate of energy dissipation. The Euler-Lagrange equations obtained using helicity balance as a constraint are solved to determine the current and magnetic field profiles of the relaxed states.

Brazilian Journal of Physics 32[1], 65-75. 2002.

P 055-02 "Tokamak NOVA-UNICAMP recent results".

Daltrini, A. M., Machida, M., Monteiro, M. J. R., and Kaminishikawahara, C. O.

Tokamak NOVA-UNICAMP is a small tokamak with iron core and conducting shell stabilization built to study plasma-wall interaction and optical diagnostic development. Characteristic plasma behavior was the appearance of 2-3 kHz spike oscillation during entire discharge with very high X-ray activity which prevent our optical diagnostic development. By modifying capacitance and charging voltage on OH and vertical field banks, in order to obtain similar discharge current shape, most of 2-3 kHz spikes has been taken out, although some activities still remains to be analyzed. Nevertheless, the high X-ray

activity which jeopardize our optical measurements is completely eliminated and time varying parameter as ion temperature is now possible to be followed during whole discharge

Brazilian Journal of Physics 32[1], 26-29. 2002.

P 056-02 "Total reflection by synchrotron radiation: trace determination in nuclear materials".

Simabuco, S. M., Vazquez, C., Boeykens, S., and Barroso, R. C.

The chemical control of impurities in nuclear materials is indispensable in order to ensure efficient operation of the reactors. The maximum concentration admitted depends on the elements and in most cases is in the parts per billion range. Conventional analytical methods require a preconcentration treatment of the sample and a previous separation of the matrix (uranium). In this work, we investigated the use of total reflection x-ray fluorescence with synchrotron radiation excitation as an alternative methodology for the determination of impurities in nuclear materials, namely K, Ca, Ti, Cr, Mn, Fe, Ni, Cu and As. The detection limits obtained were in the range 0.1-20 ng ml⁻¹) for a 1000 s counting time. Copyright (C) 2002 John Wiley Sons, Ltd

X-Ray Spectrometry 31[2], 167-172. 2002.

P 057-02 "Virial theorem and scaling of shallow-donor binding energy in quantum-sized semiconductor heterostructures".

Dios-Leyva, M. and Oliveira, L. E.

The variational and fractional-dimensional space approaches are used in a thorough study of the virial theorem value and scaling of the shallow-donor binding energies versus donor Bohr radius in $\text{GaAs}/(\text{Ga,Al})\text{As}$ semiconductor quantum wells (QWs) and quantum-well wires (QWWs). In the case of the fractional-dimensional space approach, in which the three-dimensional actual anisotropic semiconductor heterostructure is modelled by a fractional-dimensional isotropic effective medium, we have shown that if the ground-state wave function may be approximated by a D-dimensional hydrogenic wave function, the virial theorem value equals 2 and the scaling rule for the donor binding energy versus Bohr radius is hyperbolic, both for $\text{GaAs}/(\text{Ga,Al})\text{As}$ wells and wires. In contrast, calculations within the variational scheme show that the scaling of the donor binding energies with quantum-sized Bohr radius is in general nonhyperbolic and that the virial theorem value is nonconstant. Moreover, calculations for the donor binding energies versus well widths or wire radii, within both the fractional-dimensional and the variational approaches, indicate that any general conclusion based on a given virial theorem value or donor energy versus Bohr radius scaling rule should be examined with caution

Journal of Physics-Condensed Matter 13[42], 9471-9479. 2001.

Abstracta

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Publicação

Biblioteca do Instituto de Física Gleb Wataghin

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Projeto Gráfico

ÍgneaDesign

Impressão

Gráfica Central - Unicamp

